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GUNZBURGER, MAX D.

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14. ABSTRACT
We have developed novel, effective, robust algorithms that were subjected to mathematically rigorous analyses and extensive computational testing for uncertainty quantification problems of several types that involve high a high number of random variables as inputs to complex systems described by partial differential equations. The approaches developed result in superior means for science-based risk assessment and policy decision making, for simulating fluid flows and structures and other physical systems that are subject to uncertainties and for which the accurate determination of output uncertainties is crucial to the design of devices and strategies in many applications. In our efforts, we have not only availed ourselves of the latest computational and mathematical tools to design our robust, efficient, and accurate methodologies, but we have also invented several new tools for this purpose that are already been used by other researchers. Included in the latter category are multilevel stochastic collocation methods, hyperspherical transformations for discontinuity detection, transformation methods that replace difficult to treat uncorrelated random fields by correlated ones, and hierarchical approaches for improving filtering and Baysean inference problems.

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Final Report for AFOSR Grant FA9550-11-1-0149
PI: Max Gunzburger (Florida State University)

Research projects and related publications completed

G. ZHANG AND M. GUNZBURGER, *Error analysis of stochastic collocation method for parabolic partial differential equations with random input data*; SIAM Journal on Numerical Analysis, 50, 2012, 1922-1940.

A stochastic collocation method for solving linear parabolic partial differential equations with random coefficients, forcing terms, and initial conditions was analyzed. The input data were assumed to depend on a finite number of random variables. Unlike previous analyses, a wider range of situations were considered, including input data that depend nonlinearly on the random variables and random variables that are correlated or even unbounded. We provided a rigorous convergence analysis and demonstrated the exponential decay of the interpolation error in the probability space for both finite element semidiscrete spatial discretizations and for finite element, CrankNicolson fully discrete space-time discretizations. Ingredients in the convergence analysis include the proof of the analyticity, with respect to the probabilistic parameters, of the semidiscrete and fully discrete approximate solutions. A numerical example is provided to illustrate the analyses.

$\Longrightarrow$ *We provided the first rigorous analysis of stochastic collocation methods for parabolic PDE with random inputs.*

J. MING AND M. GUNZBURGER, *Efficient numerical methods for stochastic partial differential equations through transformation to equations driven by correlated noise*; International Journal for Uncertainty Quantification, 3 2013, 321-339.

A procedure was provided for the efficient approximation of solutions of a broad class of stochastic partial differential equations (SPDEs), that is, partial differential equations driven by additive white noise. The first step was to transform the given SPDE into an equivalent SPDE driven by a correlated random process, specifically, the Ornstein-Uhlenbeck process. This allowed for the use of truncated Karhunen-Love expansions and sparse-grid methods for the efficient and accurate approximation of the input stochastic process in terms of few random variables. Details of the procedure were given and its efficacy was demonstrated through computational experiments involving the stochastic heat equation and the stochastic Navier-Stokes equations.

$\Longrightarrow$ *We provided a very efficient means for treating PDEs driven by white noise which typically require a much larger number of solutions of the PDE to build accurate statistical ensembles.*

G. ZHANG, M. GUNZBURGER, AND W. ZHAO, *A sparse-grid method for multi-dimensional backward stochastic differential equations*; Journal of Computational Mathematics, 31, 2013, 221-248.

A sparse-grid method for solving multi-dimensional backward stochastic differential equations (BSDEs) based on a multi-step time discretization scheme previously developed by some of the authors was developed. In the multi-dimensional spatial domain, i.e. the Brownian space, the conditional mathematical expectations derived from the original equation were approximated using sparse-grid Gauss-Hermite quadrature rule and (adaptive) hierarchical sparse-grid interpolation. Error estimates were proved for the proposed fully-discrete scheme for multi-dimensional BSDEs with certain types of simplified generator functions. Finally, several numerical examples were provided to illustrate the accuracy and efficiency of our scheme.

$\Longrightarrow$ *In many situations, BSDEs provide an efficient means for solving deterministic PDEs by solving a simpler, albeit stochastic, differential equation. In this work, we provided a novel and very efficient (relative* *to existing approaches) for solving BSDEs.*

M. D'ELIA AND M. GUNZBURGER, *Coarse-grid sampling interpolatory methods for approximating Gaussian random fields*; SIAM/ASA Journal on Uncertainty Quantification, 1, 2013, 270-296.

Random fields can be approximated using grid-based discretizations of their covariance functions followed by, e.g., an eigendecomposition (i.e., a KarhunenLo‘eve expansion) or a Cholesky factorization of the resulting covariance matrix. We considered Gaussian random fields and analyzed the efficiency gains obtained by using low-rank approximations based on constructing a coarse grid covariance matrix, followed by either an eigendecomposition or a Cholesky factorization of that matrix, followed by interpolation from the coarse grid onto the fine grid. The result is coarser sampling and smaller decomposition or factorization problems than that for full-rank approximations. Using one-dimensional experiments, we examined the relative merits, with respect to accuracy achieved for the same computational complexity, of the different low-rank approaches. We found that interpolation from the coarse grid combined with the Cholesky factorization of the coarse grid covariance matrix yields the most efficient approach. Of course, these approaches rely on knowing the correlation function of the random field. When that function is not known (which is often the case), we explore the use of only interpolation from a coarse grid onto a fine grid as an alternative to what is usually done, which is assuming a covariance function. Computational tests performed on one- and two-dimensional uniform and nonuniform grids indicated that this approach, which does not require any matrix factorizations or decompositions, resulted in correlations that can be very similar to those that result from assuming well-known, e.g., exponential-type, correlation functions.

$\Longrightarrow$ *We developed grid-based methods for dicretizing correlated random fields which can be implemented in much the same simple way as for the ubiquitously used grid-based methods for white noise fields.*

A. LABOVSKY AND M. GUNZBURGER, *An efficient and accurate method for the identification of the most influential random parameters appearing in the input data for PDEs*; SIAM/ASA Journal on Uncertainty Quantification, 2, 2014, 82-105.

Cut-HDMR expansions (also referred to as anchored-ANOVA expansions) have often been used to represent multivariate functions in high dimensions because they can be used to identify unimportant variables. Past efforts in this direction have examined only the separate influence of each variable. However, we showed, using simple examples, that variables that have small separate influences can have large interactions, and thus those variables should not be ignored. We developed a methodology for determining the importance of variables by examining both their separate and pairwise effects. As a result, not only were all unimportant terms omitted from the cut-HDMR expansion, but all important terms were retained. This is in contrast to existing methods that can omit important pairwise interaction terms. The application and effectiveness of the new methodology were demonstrated for a nonlinear system of partial differential equations having random inputs; specifically, we considered a magnetohydrodynamics setting which also serves to illustrate that a realistic problem can indeed involve random input parameters that have small individual influences but large pairwise influences. In such settings, the new method is not only computationally attractive, but it is the only method that can correctly identify all important individual effects and pairwise interactions. Also considered is a possible further application of the new methodology, namely reducing the cost of sparse-grid approximations of quantities of interest that depend on the solution of a partial differential equation.

$\Longrightarrow$ *Reducing the number of random parameters that one must deal with in problems described by PDEs with random inputs is of paramount importance for reducing the very high costs associated with uncertainty quantification for such cases. In this work, we provided the first means for correctly identifying this parameters that are important not just in their separate effect, but also in their pairwise interactions. An algorithm* *to do this was developed and tested and applied to an MHD problem.*

M. GUNZBURGER, C. WEBSTER, AND G. ZHANG, *Stochastic finite element methods for partial differential equations with random input data*; Acta Numerica, 23, 2014, 521-650.

⟹ *Acta Numerica has for over 20 years been the leading outlet for publishing timely review articles on all aspects of computational mathematics and numerical analysis. It has been especially used to acquaint readers with emerging areas of research. I was invited to prepare and article on uncertainty quantification which is absolutely an emerging areas in mathematics and applications. The result was this 130 page article with provides a wealth of rigorous theoretical and practical useful knowledge about uncertainty quantification involving PDEs.*

C. WEBSTER, G. ZHANG, AND M. GUNZBURGER, *An adaptive sparse-grid iterative ensemble Kalman filter approach for parameter field estimation*; International Journal of Computer Mathematics, 91, 2014 798-817.

A new sparse-grid (SG) iterative ensemble Kalman filter (IEnKF) approach was developed for estimating spatially varying parameters. The adaptive high-order hierarchical sparse-grid (aHHSG) method was adopted to discretize the unknown parameter field. An IEnKF was used to explore the parameter space and estimate the surpluses of the aHHSG interpolant at each SG level. Moreover, the estimated aHHSG interpolant on coarser levels is employed to provide a good initial guess of the IEnKF solver for the approximation on the finer levels. The method is demonstrated in estimating permeability field in flows through porous media.

⟹ *By combining hierarchical sparse grids with iterative ensemble Kalman filtering, both effective in some respects in their own right, we have developed a very efficient method for parameter field estimation.*

M. GUNZBURGER AND C. WEBSTER, *Uncertainty quantification in the partial differential equation setting*; to appear in Mathematical Intelligencer.

⟹ *The Mathematical Intelligencer, published by Springer, is the leading organ, on the worldwide stage, for providing information about developments and trends in all of mathematics. I was invited to prepare this article on uncertainty quantification, arguably the hottest trend in applied mathematics and statistics.*

G. ZHANG, C. WEBSTER, AND M. GUNZBURGER, *A hyper-spherical adaptive method for discontinuity detection*; submitted.

We developed and analyzed a hyper-spherical adaptive hierarchical sparse-grid method for detecting jump discontinuities of functions in high-dimensional spaces. The method was motivated by the theoretical and computational inefficiencies of well-known adaptive sparse-grid methods for discontinuity detection. Our novel approach constructed, using a hyper-spherical transformation, a function representation of the discontinuity hyper-surface of an N-dimensional discontinuous quantity of interest. Then, a sparse-grid approximation of the transformed function, built in the hyper-spherical coordinate system, whose value at each point was estimated by solving a one-dimensional discontinuity detection problem. Due to the smoothness of the hyper-surface, the new technique could identify jump discontinuities with significantly reduced computational cost, compared to existing methods. Moreover, hierarchical acceleration techniques were also incorporated to further reduce the overall complexity. Rigorous complexity analyses of the new method were provided as were several numerical examples that illustrates the effectiveness of the approach.

⟹ *The notoriously difficult problem of discontinuity detection with respect to dependences on random parameters is the crucial task one faces in many risk assessment, policy decision, and other uncertainty quantification settings. Or approach, which does not make the futile attempts trying to identify discontinu-*

ities in parameter space, but rather does so in a transformed space, provides a novel and more effective approach for discontinuity detection.

A. TECKENTRUP, P. JANTSCH, C. WEBSTER, AND M. GUNZBURGER, *A multilevel stochastic collocation method for partial differential equations with random input data*; submitted.

Stochastic collocation methods for approximating the solution of PDEs with random input data (e.g., coefficients and forcing terms) suffer from the curse of dimensionality whereby increases in the stochastic dimension cause an explosion of the computational effort. We developed and analyzed a multilevel version of the stochastic collocation method that, as was the case for multilevel Monte Carlo (MLMC) methods, used hierarchies of spatial approximations to reduce the overall computational complexity. In addition, our proposed approach utilized, for approximation in stochastic space, a sequence of multi-dimensional interpolants of increasing fidelity which were then used for approximating statistics of the solution as well as for building high-order surrogates featuring faster convergence rates. A rigorous convergence and computational cost analysis of the new multilevel stochastic collocation method was provided, demonstrating its advantages compared to standard single-level stochastic collocation approximations as well as MLMC methods. Numerical results were provided that illustrate the theory and the effectiveness of the new multilevel method.

$\Longrightarrow$ *Mutilevel methods, e.g., multi grid methods, have historically been shown to provide avenues for great improvement in the efficiency of numerical algorithms. Our approach that combines hierarchies of spatial approximation and sparse-grid approximations in parameter space greatly improve the efficiency of solving PDEs with random inputs.*

M. GUNZBURGER AND A. TECKENTRUP, *Optimal point sets for total degree polynomial interpolation in moderate dimensions*; submitted.

Lagrange interpolation by total degree polynomials in moderate dimensions was the focus of this project. In particular, we were interested in characterizing the optimal choice of points for the interpolation problem, where we defined the optimal interpolation points as those which minimize the Lebesgue constant. We developed a novel algorithm for numerically computing the location of the optimal points, which was independent of the shape of the domain and does not require computations with Vandermonde matrices. We performed a numerical study of the growth of the minimal Lebesgue constant with respect to the degree of the polynomials and the dimension, and so produced the lowest values known as yet of the Lebesgue constant in the unit cube and the unit ball in up to 10 dimensions.

$\Longrightarrow$ *For passive approximation, i.e., barring the use of adaptive strategies, total degree polynomial interpolation provides the most efficient means for providing approximations of a desired precision. We have overcome the difficulties faced with producing a good set of interpolation points and, in fact, produced a means for determining optimal interpolations points.*

H.-W. VAN WYK, M. GUNZBURGER, J. BURKARDT, AND M. STOYANOV, *Power-law noises over general spatial domains and on non-standard meshes*; submitted.

Power-law noises abound in nature and have been observed extensively in both time series and spatially varying environmental parameters. Although recent years have seen the extension of traditional stochastic partial differential equations to include systems driven by fractional Brownian motion, spatially distributed scale-invariance has received comparatively little attention, especially for parameters defined over non-standard spatial domains. Our work focused on the generalization of power-law noises to arbitrary multidimensional spatial domains by establishing their their theoretical underpinnings as well as addressing their numerical simulation. Three computational algorithms were developed for efficiently generating their sample paths, accompanied by numerous numerical illustrations.

$\Longrightarrow$ *White noise random fields are in ubiquitous use in practice for modeling uncertainty in complex systems, despite the fact that the have infinite variance. On the other hand, power-law noises have been often observed but are difficult to simulate in eve two and three spatial dimension. We have developed efficient means for doing so.*

G. ZHANG, W. ZHAO, C. WEBSTER, AND M. GUNZBURGER, *Numerical solution of backward stochastic differential equations with jumps for a class of nonlocal diffusion problems*; submitted.

We developed a novel numerical approach for linear nonlocal diffusion equations with integrable kernels, based on the relationship between the backward Kolmogorov equation and a class of backward stochastic differential equations (BSDEs) driven by Lèvy processes with jumps. The nonlocal diffusion problem under consideration was converted into a BSDE, for which numerical schemes were developed and applied directly. The most significant advantage of our approach is that the BSDE can be solved independently along each trajectory of the underlying Lèvy processes, and therefore, completely avoids the difficulties associated with solving sequences of linear systems required by traditional numerical approximations. In addition, the inherent independence of our procedure allows for embarrassingly parallel implementations and also enables adaptive approximation techniques to be incorporated in a straightforward fashion. Rigorous error analysis of the new method were developed as were several numerical examples that illustrated the effectiveness and efficiency of the proposed approach.

$\Longrightarrow$ *Standard discretization of nonlocal diffusion problems result in matrices that significantly less sparse than the corresponding discretizations of PDEs. Our approach completely avoids the need to solve matrix problems, so that it provides and efficient means for solving nonlocal diffusion problems.*

G. ZHANG, D. LU, M. YE, M. GUNZBURGER, AND C. WEBSTER, *An adaptive sparse-grid high-order stochastic collocation method for Bayesian inference in groundwater reactive transport modeling*; Water Resources Research, 49, 2013, 1-22.

Bayesian analysis has become vital to uncertainty quantification in groundwater modeling, but its application has been hindered by the computational cost associated with numerous model executions required to explore the posterior probability density function (PPDF) of model parameters. This is particularly the case when the PPDF is estimated using Markov Chain Monte Carlo (MCMC) sampling. We developed a new approach to improve the computational efficiency of Bayesian inference by constructing a surrogate of the PPDF, using an adaptive sparse-grid high-order stochastic collocation (aSG-hSC) method. Unlike previous works using first-order hierarchical bases, our approach utilized a compactly supported higher-order hierarchical basis to construct the surrogate system, resulting in a significant reduction in the number of required model executions. In addition, using the hierarchical surplus as an error indicator allowed locally adaptive refinement of sparse grids in the parameter space, which further improved computational efficiency. To efficiently build the surrogate system for the PPDF with multiple significant modes, optimization techniques were used to identify the modes, for which high-probability regions were defined and components of the aSG-hSC approximation were constructed. After the surrogate was determined, the PPDF can be evaluated by sampling the surrogate system directly without model execution, resulting in improved efficiency of the surrogate-based MCMC compared with conventional MCMC. The developed method was evaluated using two synthetic groundwater reactive transport models. The first example involved coupled linear reactions and demonstrated the accuracy of our high-order hierarchical basis approach for approximating high-dimensional posteriori distribution. The second example was highly nonlinear because of the reactions of uranium surface complexation, and demonstrated how the iterative aSG-hSC method was able to capture multimodal and non-Gaussian features of PPDF caused by model nonlinearity. Both experiments showed that aSG-hSC is an effective and efficient tool for Bayesian inference.

$\Longrightarrow$ *Although our novel approach was developed in the context of groundwater flow modeling, the algorithmic innovations apply to many other Baysean inference setting.*

J. CHOI AND M. GUNZBURGER, *Approximation and application of the Musiela stochastic PDE in forward rate models*; International Journal of Computer Mathematics, 89, 2012, 1269-1280.

We considered the Musiela equation of forward rates; this is a hyperbolic stochastic partial differential equation. A weak formulation of the problem using the streamline upwind PetrovGalerkin method was analysed. Error analyses of the method yielded estimates for the convergence rates. Computational examples were provided that illustrated not only the discretization methods used, but the type of results relevant to bond pricing that can be obtained from the equation.

$\Longrightarrow$ *Our rigorously justified methodologies provide a superior means for approximating forward rate models*

Personnel (partially) supported

Senior investigator

Max Gunzburger (PI)

Postdoctoral researchers

Marta D'Elia (now at Sandia National Laboratories)

Aretha Teckentrup (now at the University of Bath in the United Kingdom)

Ju Ming (now at the Beijing Center for Computational Mathematics)

Hans-Werner von Wyk (current a postdoc at FSU)

Students

Qingguang Guan (current a student at FSU)

Michael Schneier (current a student at FSU)

Guannan Zhang (now at the Oak Ridge National Laboratory)